Synopsis

on

"Relaxation Dynamics in Biomolecules: A Dielectric and Thermodynamic approach using TDR

Submitted

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RELAXATION DYNAMICS IN BIOMOLECULES: A DIELECTRIC AND THERMODYNAMIC APPROACH USING TDR

INTRODUCTION:

Biomolecules and biopolymers play an important role in physical, chemical and biological processes and are very important class of organic compounds. A biomolecule is that molecule which is present in living organisms, including large macromolecules such as **proteins, carbohydrates, polysaccharides, lipids, and nucleic acids**, as well as small molecules such as primary metabolites, secondary metabolites, and natural products. Most of biomolecules are organic compounds. Many biological systems such as proteins and enzymes are inactive without water. For the complete knowledge about the function of such systems, understanding of the **structure and dynamics** of the aqueous environment surrounding the concerned biomolecule is essential [1].

The dielectric relaxation study at microwave frequency gives information about solute-solvent and protein-legand interaction [2]. The present study is to report the relaxation dynamics of some biomolecules using **Time Domain Reflectometry (TDR)** in the temperature range 0^0C to 25^0C over the frequency region of 10 MHz- 20 GHz or less. The information related to the solute-solvent/protein-legand interaction in biomolecules has been carried out and expressed in terms of **static dielectric permittivity and relaxation time and the results may be verified through thermodynamic parameters like free energy of activation, entropy of activation and enthalpy of activation**. Time Domain Reflectometry (TDR) Technique in reflection mode has been used to measure dielectric parameters viz. Dielectric loss, Static dielectric permittivity and relaxation Time. Further, Fourier transforms and least square fit method has been used to obtain dielectric parameters. With change in concentration and temperature, the systematic changes in dielectric parameters can be studied [2].

Dielectric properties of biological macromolecules have been the subject of experimental and theoretical studies for quite longer time. These properties are greatly affected by the presence of water and other solvents to an extent that this behaviour could be used as a means of investigating the role of solvent in the various biomolecules/biopolymers. The characterization of the dielectric properties in terms of the state of hydration, concentration, frequency and temperature, might provide useful data from which the molecular processes underlying the macroscopic results could be analyzed.

Conformational transformations of biopolymers and biomolecules generally lead to substantial changes of the dielectric properties which reflect the accompanying changes of overall structure. Properties of biomolecules changes with temperature, solute-solvent concentration and other parameters. Some biomolecules and biopolymers containing oxygen atoms or –OH groups can enter into intra and/or intermolecular hydrogen bonding giving rise to several conformers in different solvents. Therefore, it is important to study the structural and dynamical behaviour of such biomolecules in its pure liquid state or in different solvents by changing its environment (concentration, temperature etc.).

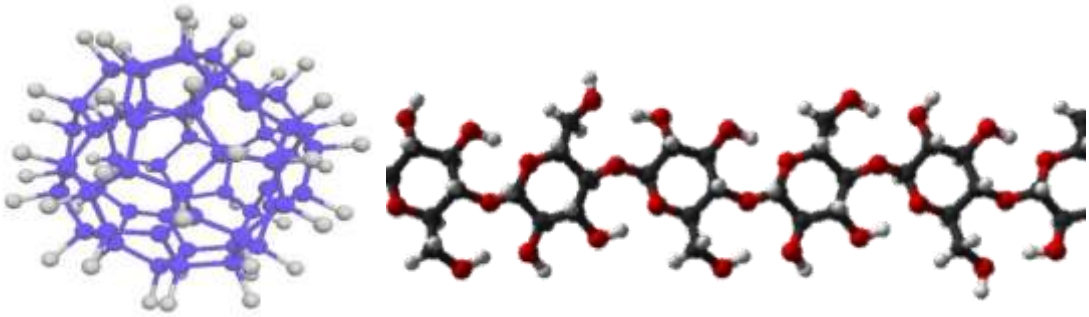

Fig.1. Biomolecules

Despite several efforts devoted to the study of investigation of structural and dynamical properties of biomolecules and biopolymers over many years, there are still many interesting aspects of **molecular interaction** and spectroscopic behaviour, which have not been understood thoroughly.

Review of literature:

Bonincontro and Risuleo [3] suggest that biomolecules exposed to an electric field in the radio frequency range (3 kHz to 300 GHz) generally show dielectric relaxation due to orientation polarization (dipole-dipole interactions). The authors are able to determine two significant parameters (the effective hydrodynamic radius and the electric dipole moment) from the dispersion curve, characterizing conformation and structure of the biomolecules. Although, supplementary knowledge on their effects on structural and dielectric behaviors of biomolecules is lacking in literature. Furthermore, regarding their electrical properties, their dielectric properties, and their sensitivity to environmental factors such as water vapor and carbon dioxide, it is hypothesized that proteins can be used as bio-sensors for the measurement of a physical, chemical, biological or any other parameter, giving a response in terms of resistance, voltage or current [4].

Many investigations demonstrated the importance of water molecules in the first layer of water shell [5] and that their properties differ from those of bulk water[6] The main reason is that a significant fraction of these water molecules may be involved in direct interactions with protein atoms, and thus their ability to move and reorient can be severely restricted in comparison with those of the bulk water[7].

Objectives of a Research:

The main objective of the proposed research work is to carry out and **study molecular interaction, structural and dynamical behaviour of some biomolecules** of low conductivity when environment of such systems i.e. temperature, concentration, number of atoms, frequency and other parameters changes. The effect of molecular weight, temperature and concentration on biomolecules will also be the thrust areas of this work while studying molecular behaviour and physical properties using different spectroscopic techniques.

Another objective of this article is to present a quantitative theory of dielectric relaxation of biomolecules based on a dynamic equilibrium between the free and bound water molecules. The theory is based on the assumption that a dynamic exchange between the free and bound molecules, controlled by the strength and the hydrogen bond in biomolecule, determines the observed dynamics [1].

Methodology to be adopted:

Various techniques are available to study the molecular interaction, structural and dynamical behavior of biomolecules and biopolymers such as Fourier Transform Infra-Red (FTIR), X-ray Nuclear Magnetic Resonance (NMR) and Dielectric spectroscopy. In the present work we will use Time Domain Reflectometry (TDR) technique to obtain information on the structural, dynamical and molecular interaction in biomolecules and biopolymers. Effect of concentration, frequency and temperature may also be included in the study. The principle of TDR is understood as a incidence of time dependent pulse and its subsequent reflection from given sample in time scale is observed and monitored by oscilloscope and change in shape and size of the pulse before and after reflection provides us important information about the nature of sample.

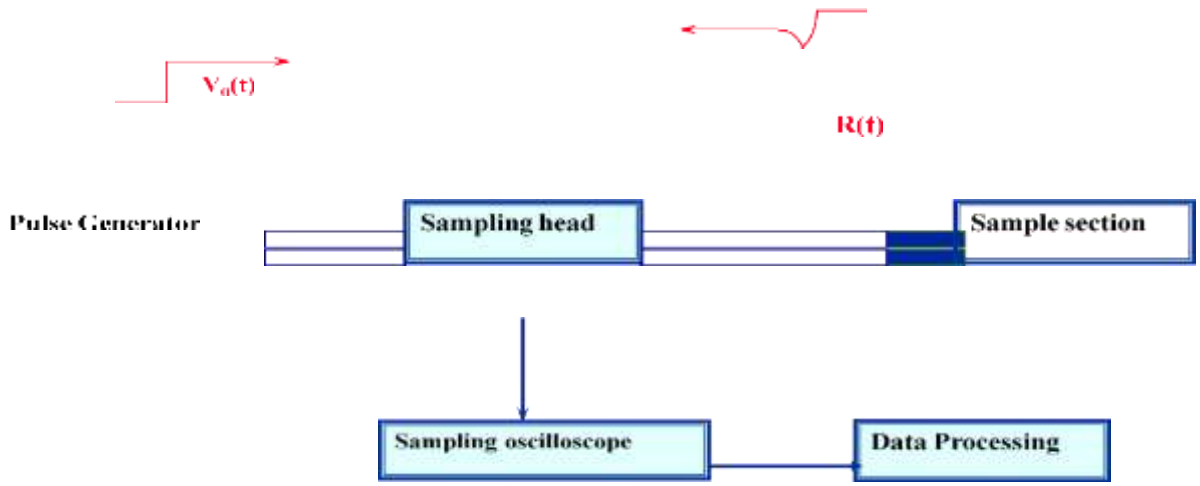

Fig.2.Principle of TDR

The block diagram and experimental set-up of TDR is as shown in Fig.2 [8].

TDR technique is used for investigation of dielectric permittivity and dielectric properties of liquid [9]. Dielectric relaxation study through TDR technique makes it possible to determine permittivity over a wide frequency range in a single measurement[10].

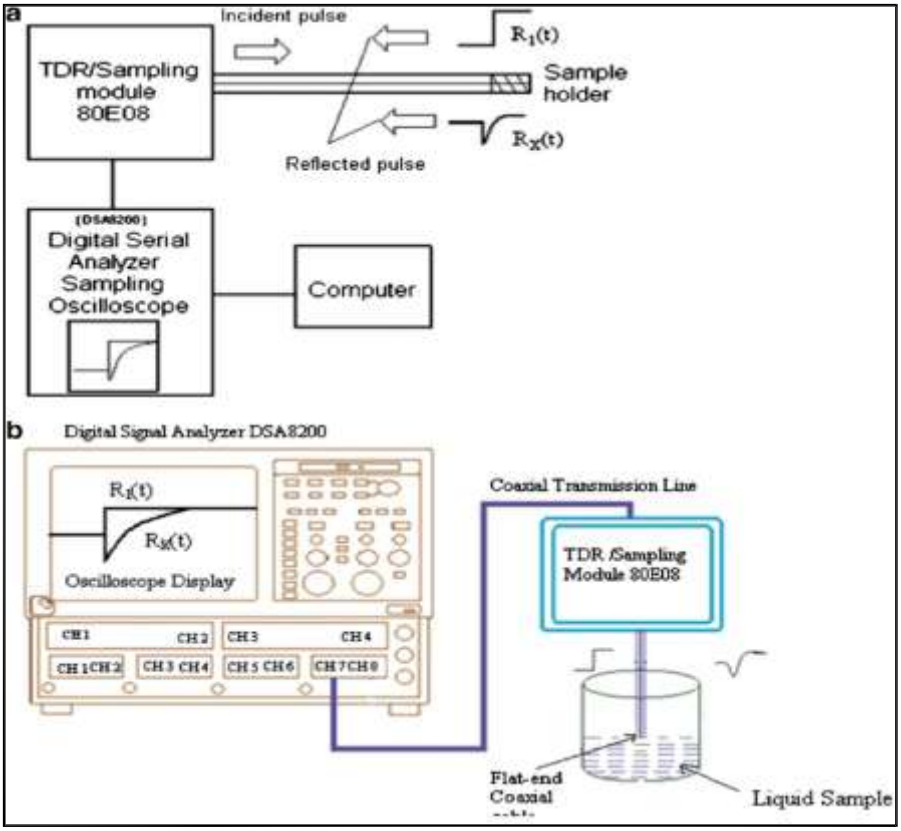

Fig. 3. (a) Block diagram of Time Domain Reflectometry (TDR). (b) Experimental setup of TDR.

TDR is used to determine the dielectric properties of the material such as Static dielectric constant (ε_0) , dielectric constant (ε'), dielectric loss (ε''), Relaxation time(τ).

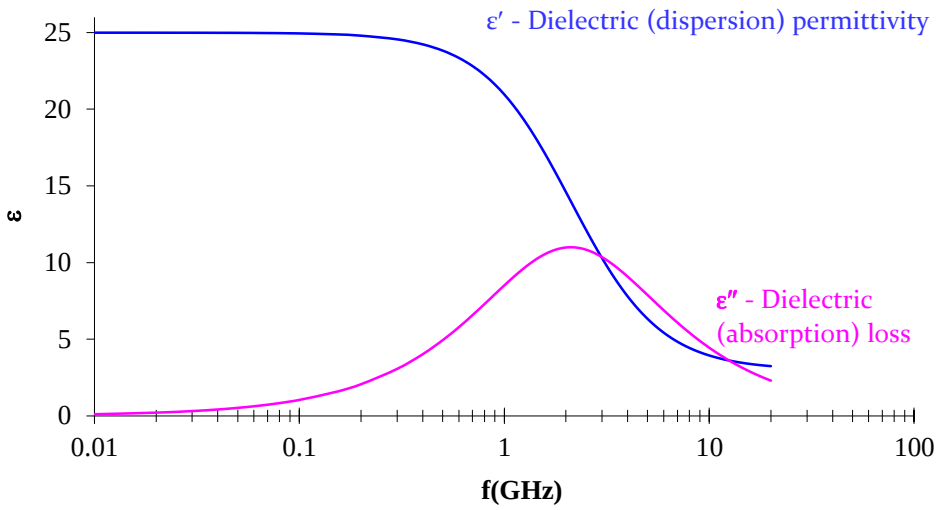

Fig.4. Time domain complex permittivity spectra for biomolecule (e.g. water)

Society applications:

Biomolecules and biopolymers find a variety of applications in every field. The applications of biomolecules are not only restricted to our life but it extends to other applications also. Recently, preparation of nanomaterial by the use of the special properties of biomolecules has gained more and more research interest. Preparation of nanomaterials with the use of biomolecules can often has some control on the morphology and size of the final products. Biomolecules are also used for the development of biosensors and their wide applications.

Because of their wide band applications in every field like science, engineering and technology, it is indeed important to look into molecular interaction, structural and dynamical properties of polymers using spectroscopic methods.

Biomolecules such as RNA, DNA, peptides, and proteins are emerging as powerful chemical tools for the **synthesis of inorganic nanoparticles**[11].

Significance of the study:

The process of molecular biology generally displays a high degree of specificity and efficiency unknown for simpler thermo physical and physicochemical phenomena. These peculiar properties can be attributed to appropriately evolved control and regulation mechanisms in which certain biomoleculs and biopolymers play a vital role. Such macromolecular compounds usually have definite conformations which are of crucial significance for their biological function therefore it will be of the greatest importance to elucidate the nature of pertinent structures and their functional potentialities. Therefore, the study of biomolecules/biopolymers will be helpful in understanding the structural and Dynamical behavior of molecules in different environment (i.e. temperature, concentration, etc.) using the dielectric parameters like dielectric permittivity, dielectric constant, relaxation time and thermo dynamical parameters such as entropy of activation, enthalpy of activation, free energy and many other physical parameters.

Proposed work plan/Formulation and Structure of study Six month wise plan of the work and target to be achieved:

First six month (Stage I):

In this first stage, we will start to build up necessary background knowledge to understand the area of my research and getting broad view about my research topics, for that we will survey the literatures like research papers, Journals, Conference Proceedings, monographs and some reference books. I will be collect samples related to my research work .I also plan to attend some useful conferences, seminars, workshops, annual foundation schools etc, and complete the course work and we will submit the first progress report at the end of sixth month..

Next six month (stage II):

In this stage, Different types of methodology, methods, and techniques will be used to determine properties or parameters of selected samples. We will focus on solving the new research problems in different forms, also in this stage we will visits some libraries, research institutes, some researchers working related to these topics for the guidance and improving the research work carried out by me as well as verifications of the research methodology, in this stage II, I will attend some useful National, International conferences, seminars, workshops during these days, and research findings will be present/publishes in the National, International conferences/Journals. Second progress report will be submitted at the end of sixth month.

Next six month (stage III):

In this third stage, the collected material will be analyzed and discover finding directions towards a research. The outcomes of my research work will be presented/ published in the National, International conferences/journals. The third progress report will be submitted at the end of stage III. Final synopsis will be submitted to the university after that writing the thesis, checking the anti-plagiarism, facing the pre-Ph.D. Viva, printing and binding the thesis will be done for submitting the thesis.

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